

Nonlinear thermal properties of three-terminal mesoscopic dielectric systems

Y. Ming*

*School of Physics and Material Science, Anhui University,
Hefei, Anhui 230039, People's Republic of China*

Z.X. Wang, Q. Li, and Z.J. Ding[†]

*Hefei National Laboratory for Physical Sciences at Microscale and
Department of Physics, University of Science and Technology of China,
Hefei, Anhui 230026, People's Republic of China*

(Dated: February 5, 2008)

Abstract

This paper studies the thermal properties of three-terminal mesoscopic dielectric systems in the nonlinear response regime at low temperature. For a symmetric three-terminal system, when the temperature is finitely different between the left and right thermal reservoir, the temperature of the central thermal reservoir is always higher than the averaging temperature of the others. This nonlinear thermal phenomenon is also observed for asymmetric three-terminal systems. At the end, a model of thermal rectification is presented.

*Electronic address: meanyee@ustc.edu

[†]Electronic address: zjding@ustc.edu.cn

With the development of the modern electronics, heat conduction, as the counterpart of electric conduction, has attracted much attention in recent years. Some research works [1, 2, 3, 4] focus on the universal quantum of thermal conductance which is predicted by Rego and Kirczenow [5] and has already been verified by experiment [6]. The quantum of thermal conductance indicates that the heat conduction is determined by the ballistic transmission of the acoustic phonon at low temperature. On the other hand, thermal rectification to control the heat flux [7, 8, 9, 10, 11, 12, 13, 14] is very interesting. Experimental work to demonstrate the thermal rectification is reported recently [15].

Based on the above efforts, this paper further studies thermal rectification in ballistic heat conduction. For heat conduction in a two-terminal mesoscopic dielectric system at low temperature, because transmission coefficients of ballistic phonons are independent on the temperature, there should be no thermal rectification[12]. But, for electric conduction within a three-terminal ballistic junction, previous investigations have indicated the nonlinear ballistic transport of electrons. That is, if voltages V_L and V_R are applied on the left and right branches of a symmetric three-terminal ballistic junction in push-pull fashion, with $V_L = -V_R$, the voltage at the central branch is always Negative [16, 17, 18, 19, 20, 21, 22]. This nonlinear property can be used for rectification, second-harmonic generation, and logic function [23, 24, 25]. Motivated by the nonlinear electrical properties in three-terminal ballistic junctions, in this work, we study the thermal properties of three-terminal mesoscopic dielectric systems in the nonlinear response regime and try to propose a model of thermal rectification. The model works at low temperature in order to keep the ballistic transmission of phonons, similar with the model taken in Ref. [14].

The geometry of the symmetric three-terminal mesoscopic dielectric system is sketched in Fig. 1. Regions $-L$, $-R$ and $-C$ are left, right and central terminals, respectively. Region $-J$ is the midsection. Assuming that the terminals are perfect and phonons coming from thermal reservoirs are not scattered within the terminals, the energy flux \dot{Q}_i from terminal i ($i = L, R, C$) flowing into the midsection J can be expressed as [26, 27]

$$\dot{Q}_i = \sum_{j(j \neq i)} \sum_m \int_{\omega_{im}}^{+\infty} [n(T_i, \omega) - n(T_j, \omega)] \hbar \omega \tau_{ji,m}(\omega) \frac{d\omega}{2\pi}, \quad (1)$$

where $n(T_i, \omega) = [\exp(\hbar\omega/k_B T_i) - 1]^{-1}$ is the Bose-Einstein distribution function of the phonons in the i th reservoir, T_i is the equilibrium temperature of thermal reservoir i , ω_{im} is the cutoff frequency of mode m in terminal i , $\tau_{ji,m}(\omega) = \sum_n \theta(\omega - \omega_{jn}) \tau_{ji,nm}$ and $\tau_{ji,nm}$ is the transmission coefficient from mode m of terminal i at frequency ω across all the interface into the mode n of terminal j .

Firstly we let the energy flux flows through the two terminals L and R and keep zero flux in terminal C (i.e. $\dot{Q}_C = 0$) and then calculate the temperature T_C . In the linear response regime, the flux in terminal C can be written as [26, 27] $\dot{Q}_C = \sum_{j=L,R} G_{jC} (T_C - T_j) = 0$, where G_{jC} is the two-terminal thermal conductance from central terminal C to terminal j ($= L$ or R). Due to the symmetry of the three-terminal mesoscopic dielectric system and the independence on the temperature of transmission coefficients, the thermal conductances from central terminal to left terminal and right terminal are equal, i.e. $G_{LC} = G_{RC}$. So the temperature of central thermal reservoir in the linear response regime is simply the averaging temperature of the left and the right thermal reservoirs, i.e. $T_C = (T_L + T_R)/2$.

When the system is not in the linear response regime and with the finite temperature difference of $2|\Delta T|$ between the left thermal reservoir and the right thermal reservoir, what is the temperature T_C of the central thermal reservoir? To figure out it, we let $T_L = T_0 + \Delta T$ and $T_R = T_0 - \Delta T$. By using the Taylor expansion of the Bose-Einstein distribution function $n(T_i, \omega)$, when $|\Delta T|$ is a small value, the temperature T_C can be written as

$$T_C = T_0 + \frac{1}{2}\alpha(\Delta T)^2 + \mathcal{O}[(\Delta T)^4], \quad (2)$$

where

$$\alpha = \frac{\sum_m \int_{\omega_{Cm}}^{+\infty} \left(\frac{\partial^2 n(T, \omega)}{\partial T^2} \right)_{T_0} \hbar \omega \tau_{LC,m}(\omega) \frac{d\omega}{2\pi}}{\sum_m \int_{\omega_{Cm}}^{+\infty} \left(\frac{\partial n(T, \omega)}{\partial T} \right)_{T_0} \hbar \omega \tau_{LC,m}(\omega) \frac{d\omega}{2\pi}}. \quad (3)$$

Here, $\tau_{RC,m} = \tau_{LC,m}$ by the symmetry of the system and the independence on the temperature of the transmission coefficients. Thus, T_C depends quadratically on ΔT for small $|\Delta T|$. By using $e^x = \sum_{l=0}^{\infty} \frac{1}{l!} x^l$, for all $\omega > 0$, we can easily obtain that

$$\left(\frac{\partial n(T, \omega)}{\partial T} \right)_{T_0} = \frac{\hbar \omega \exp(\hbar \omega / k_B T_0)}{k_B T_0^2 [\exp(\hbar \omega / k_B T_0) - 1]^2} > 0, \quad (4)$$

$$\begin{aligned} \left(\frac{\partial^2 n(T, \omega)}{\partial T^2} \right)_{T_0} &= \frac{\hbar \omega \exp(\hbar \omega / k_B T_0)}{k_B T_0^3 [\exp(\hbar \omega / k_B T_0) - 1]^3} \\ &\times \sum_{l=3}^{\infty} \frac{l-2}{l!} \left(\frac{\hbar \omega}{k_B T_0} \right)^l > 0. \end{aligned} \quad (5)$$

Thus, it is obtained that $\alpha > 0$ and $\alpha \propto 1/T_0$ approximately. Thus $T_C > T_0 = (T_L + T_R)/2$ is always true when the temperature difference between the left and the right thermal reservoirs is finite.

Next, we will carry out numerical calculations for a three-terminal system shown in Fig. 1. The scalar model for the elastic wave is considered. And the model for thin geometry at low

temperature is used so that the calculation is two-dimensional. So we can derive the transmission coefficient, $\tau_{ji,m}$, by the scattering matrix method [26, 28, 29]. In the calculation, we employ the following values of elastic stiffness constant and the mass density for GaAs[30]: $C_{44} = 5.99 \times 10^{10} \text{ Nm}^{-2}$ and $\rho = 5317.6 \text{ kgm}^{-3}$, and choose $W_L = W_R = 10 \text{ nm}$, $W_T = 20 \text{ nm}$ and $W_C = D_J = 10 \text{ nm}$. We truncate the sum of m in Eq. (1) at $m = 10$ [29] and limit the temperatures of the left and the right thermal reservoirs lower than $T_{ph} = \hbar\pi v/W_L k_B \approx 7.61 \text{ K}$ ($v = \sqrt{C_{44}/\rho}$ is the sound velocity). At this low temperature, the phonon relaxation can be neglected [26] and the heat conduction is mainly determined by the ballistic transmission of the acoustic phonons.

Fig. 2 shows $T_C - T_0$ vs ΔT for four different T_0 s, where T_0 is the averaging value of T_L and T_R , and $T_L = T_0 + \Delta T$, $T_R = T_0 - \Delta T$. First, it can be seen that when the difference between T_L and T_R is finite ($|\Delta T| > 0$), the temperature of the central thermal reservoir T_C is always higher than the averaging value of T_L and T_R , i.e. $T_C - T_0 > 0$, no matter which thermal reservoir has the higher temperature. Second, the temperature T_C shows a quadratic dependence on ΔT , in agreement with Eq. (2). Third, as mentioned above that $\alpha \propto 1/T_0$ approximately, the curvatures of the curves depend strongly on the temperature T_0 . The lower the temperature T_0 , the larger the curvature.

To study the nonlinear properties in the asymmetric three-terminal systems, we let the energy flux flows through the two terminals L and C and keep zero flux in terminal R (i.e. $\dot{Q}_R = 0$) and then calculate the temperature T_R . Same as Eq. (2), with $\tau_{CR,m} > \tau_{LR,m}$, the temperature T_R can be written as

$$T_R = T_0 - \beta(\Delta T) + \frac{1}{2}\gamma(\Delta T)^2 + O[(\Delta T)^3], \quad (6)$$

where

$$\beta = \frac{\sum_m \int_{\omega_{Rm}}^{+\infty} \left(\frac{\partial n(T, \omega)}{\partial T} \right)_{T_0} \hbar \omega (\tau_{CR,m} - \tau_{LR,m}) \frac{d\omega}{2\pi}}{\sum_m \int_{\omega_{Rm}}^{+\infty} \left(\frac{\partial n(T, \omega)}{\partial T} \right)_{T_0} \hbar \omega (\tau_{CR,m} + \tau_{LR,m}) \frac{d\omega}{2\pi}} > 0, \quad (7)$$

$$\gamma = \frac{\sum_m \int_{\omega_{Rm}}^{+\infty} \left(\frac{\partial^2 n(T, \omega)}{\partial T^2} \right)_{T_0} \hbar \omega (\tau_{CR,m} + \tau_{LR,m}) \frac{d\omega}{2\pi}}{\sum_m \int_{\omega_{Rm}}^{+\infty} \left(\frac{\partial n(T, \omega)}{\partial T} \right)_{T_0} \hbar \omega (\tau_{CR,m} + \tau_{LR,m}) \frac{d\omega}{2\pi}} > 0. \quad (8)$$

Fig. 3 shows $T_R - T_0$ vs ΔT for four different T_0 s. The curves are also open up parabolic, in agreement with Eq. (6). The major difference with the symmetric case is that, here $T_R - T_0$ is no longer a symmetric function of ΔT with respect $\Delta T = 0$ but respect about $\Delta T = \beta/\gamma$, and can be less than zero when $0 < \Delta T < 2\beta/\gamma$. This means for some specific positive values of ΔT , the temperature T_R can be less than the averaging value of T_L and T_C . The minimal value of T_R is about $T_0 - \beta^2/2\gamma$.

In summary, for symmetric three-terminal systems in the nonlinear response regime, we have found that the temperature of the central thermal reservoir is always higher than the averaging temperature of the left and the right thermal reservoirs. For the asymmetric three-terminal systems, the same nonlinear thermal properties can be also observed except that, in some special situations, the temperature of the central thermal reservoir can be lower than the averaging temperature of the left and the right thermal reservoirs. We would like emphasize that the temperature of the central thermal reservoir is insensitive to the details of the transmission characteristics. It is different from the electric case where the output voltage at the central branch shows fluctuations due to the transmission fluctuations[21]. This difference is due to the fact that the electric current is carried by a few electrons near the Fermi energy[31] but the heat flux is contributed by all phonons with different frequencies. The nonlinear thermal properties of the symmetric three-terminal systems can be used to control the heat flux. For example, when the temperature T_C of the central thermal reservoir is lower than the averaging temperature $(T_L + T_R)/2$ of the left and the right thermal reservoirs, it is easier that the energy flux flows into the central thermal reservoir than the energy flux flows out from the central thermal reservoir when $T_C > (T_L + T_R)/2$.

Y. Ming is supported by the Talent Group Construction Foundation of Anhui University (Grant No. 02203104/04). Z.J. Ding is supported by the National Natural Science Foundation of China (Grant No. 10574121 and 10025420), Chinese Education Ministry and Chinese Academy of Sciences.

-
- [1] W.-X. Li, K.-Q. Chen, W. Duan, J. Wu, and B.-L. Gu, Appl. Phys. Lett. **85**, 822 (2004).
- [2] W.-X. Li, T. Liu, and C. Liu, Appl. Phys. Lett. **89**, 163104 (2006).
- [3] L.-M. Tang, L.-L. Wang, K.-Q. Chen, W.-Q. Huang, and B. S. Zou, Appl. Phys. Lett. **88**, 163505 (2006).
- [4] X.-F. Peng, K.-Q. Chen, B. S. Zou, and Y. Zhang, Appl. Phys. Lett. **90**, 193502 (2007).
- [5] L. G. C. Rego and G. Kirczenow, Phys. Rev. Lett. **81**, 232 (1998).
- [6] K. Schwab, E. A. Henriksen, J. M. Worlock, and M. L. Roukes, Nature (London) **404**, 974 (2000).
- [7] M. Terraneo, M. Peyrard, and G. Casati, Phys. Rev. Lett. **88**, 094302 (2002).
- [8] B. Li, L. Wang, and G. Casati, Phys. Rev. Lett. **93**, 184301 (2004).
- [9] B. Li, J. Lan, and L. Wang, Phys. Rev. Lett. **95**, 104302 (2005).
- [10] B. Li, L. Wang, and G. Casati, Appl. Phys. Lett. **88**, 143501 (2006).
- [11] B. Hu, L. Yang, and Y. Zhang, Phys. Rev. Lett. **97**, 124302 (2006).
- [12] D. Segal and A. Nitzan, Phys. Rev. Lett. **94**, 034301 (2005).
- [13] J.-P. Eckmann and C. Mejía-Monasterio, Phys. Rev. Lett. **97**, 094301 (2006).
- [14] G. Casati, C. Mejía-Monasterio, and T. Prosen, Phys. Rev. Lett. **98**, 104302 (2007).
- [15] C. W. Chang, D. Okawa, A. Majumdar, and A. Zettl, Science **314**, 1121 (2006).
- [16] K. Hieke and M. Ulfward, Phys. Rev. B **62**, 16727 (2000).
- [17] H. Q. Xu, Appl. Phys. Lett. **78**, 2064 (2001).
- [18] I. Shorubalko, H. Q. Xu, I. Maximov, P. Omling, L. Samuelson, and W. Seifert, Appl. Phys. Lett. **79**, 1384 (2001).
- [19] L. Worschech, H. Q. Xu, A. Forchel, and L. Samuelson, Appl. Phys. Lett. **79**, 3287 (2001).
- [20] D. Csontos and H. Xu, J. Phys.: Condens. Matter **14**, 12513 (2002).
- [21] D. Csontos and H. Xu, Phys. Rev. B **67**, 235322 (2003).
- [22] D. Wallin, I. Shorubalko, H. Q. Xu, and A. Cappy, Appl. Phys. Lett. **89**, 092124 (2006).
- [23] H. Q. Xu, Appl. Phys. Lett. **80**, 853 (2002).
- [24] I. Shorubalko, H. Q. Xu, P. Omling, and L. Samuelson, Appl. Phys. Lett. **83**, 2369 (2003).
- [25] L. Worschech, D. Hartmann, S. Reitzenstein, and A. Forchel, J. Phys.: Condens. Matter **17**, R775 (2005).
- [26] Q. F. Sun, P. Yang, and H. Guo, Phys. Rev. Lett. **89**, 175901 (2002).

- [27] P. Yang, Ph.D. thesis, McGill University (2004).
- [28] W. D. Sheng, J. Phys.: Condens. Matter **9**, 8369 (1997).
- [29] Y. Ming, Z. X. Wang, and Z. J. Ding, Phys. Lett. A **350**, 302 (2006).
- [30] K. Q. Chen, X. H. Wang, and B. Y. Gu, Phys. Rev. B **61**, 12075 (2000).
- [31] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1997).

Figure Captions:

Fig. 1. Schematic illustration of a symmetric three-terminal mesoscopic dielectric system.

Fig. 2. $T_C - T_0$ vs ΔT , calculated for a three-terminal system shown in Fig. 1, for four different averaging temperatures, $T_0 = (T_L + T_R)/2$, where T_C , T_L and T_R are the temperatures of the central, the left and the right thermal reservoirs, respectively. All the temperatures are reduced by $T_{ph} \approx 7.61$ K.

Fig. 3. $T_R - T_0$ vs ΔT , calculated for a three-terminal system shown in Fig. 1, for four different temperatures, $T_0 = (T_L + T_C)/2$, where T_C , T_L and T_R are the temperatures of the central, the left and the right thermal reservoirs, respectively. All the temperatures are reduced by $T_{ph} \approx 7.61$ K.

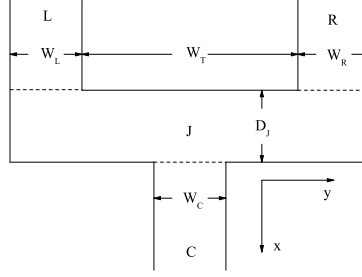


FIG. 1:

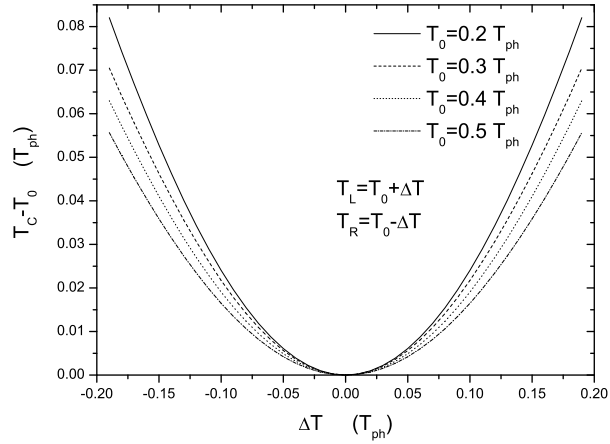


FIG. 2:

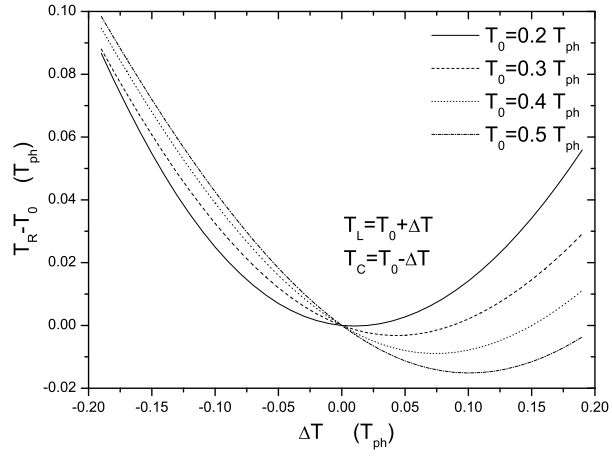


FIG. 3: